The theory and computation programs
Highlights, challenges, plans

Presented by invitation of the

Theory Coordinating Committee

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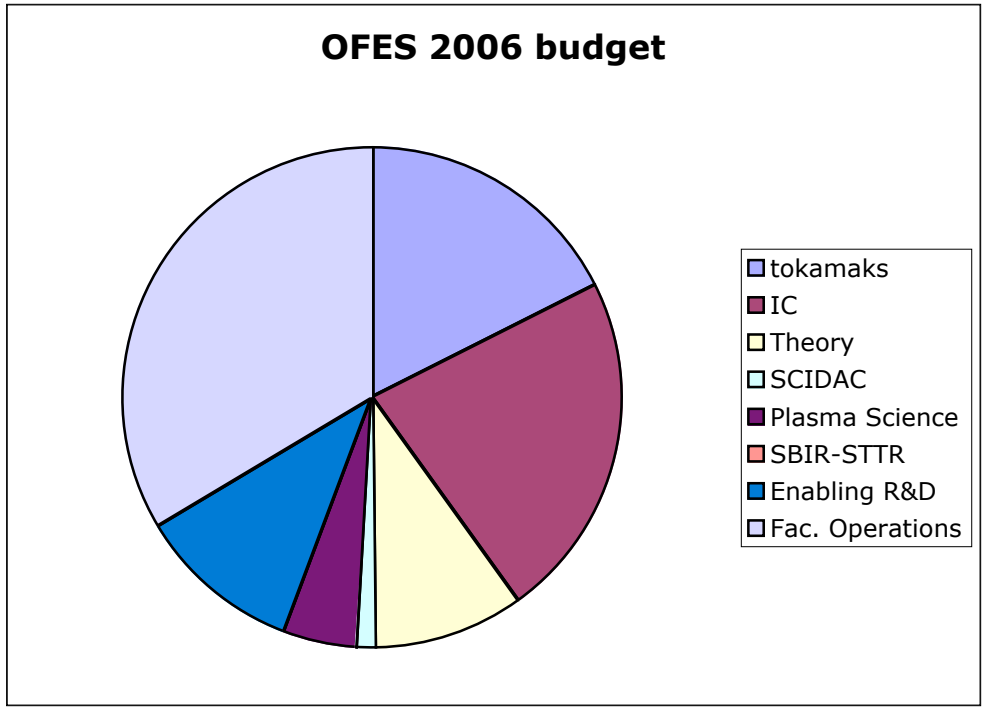
Institute for Fusion Studies, University of Texas at Austin

DOE/OFES Budget Planning Meeting
Gaithersburg, MD, March 15 & 16, 2005

Outline

- Introduction and overview of theory program management
- A sampling of recent accomplishments
- Issues and challenges

Theory and computation constitute 10% of the 2006 request



What is the role of theory within the fusion program?

The theory/computing program supplies *prediction tools*.

Why do we need a separate theory program?

- T/C research requires long term investments
- T/C research is inherently device-independent

Note that

- The concept of deliverables is of limited usefulness in managing science programs such as the T/C program. This makes management challenging.

How do we make the case for investing in Theory/Comp?

OMB/OSTP R&D Investment Criteria:

	Quality	Relevance	Performance
Prospective	COV Review (Nevins)	FESAC, NRC-BP(Ahearne-Fonck), ITPA, TCC, ECC	
	[1] Mechanism of Award [2] Justification of funding distribution among classes of performers	Planning & Prioritization	"Top N" Milestones (5 < N < 10)
Retrospective	FESAC (Sheffield), NRC reviews		
	[1] Expert reviews of successes and failures [2] Information on major awards	Evaluation of utility of R&D results to both field and broader "users"	Report on "Top N" Milestones

Recommendations of the FESAC theory panel (Sheffield)

"The panel (…) acknowledges that theory and computing in fusion energy sciences has a stellar record of research successes."

It recommended:

1. More systematic management procedure needed
   - IPPA + Vision statement, enhanced role for TCC
   - T/C support should be included in proposals for experiments
   - Manage the code supply, avoid duplication
2. Continue to strengthen advanced computing
3. Enhance connectivity with non-fusion science
4. Resist separation of theory, computing, modeling
5. Attract and retain young scientists
6. Improve peer review:
   - provide rewards for collaborations with experiment and involvement in cross-institutional teams;
   - incorporate relevance to the US program and stature in the international program as criteria.

Recommendations of the COV panel (Nevins)

"The COV was pleased to conclude that the research portfolio supported by the OFES Theory and Computations Program was of very high quality."

The COV recommended that OFES:

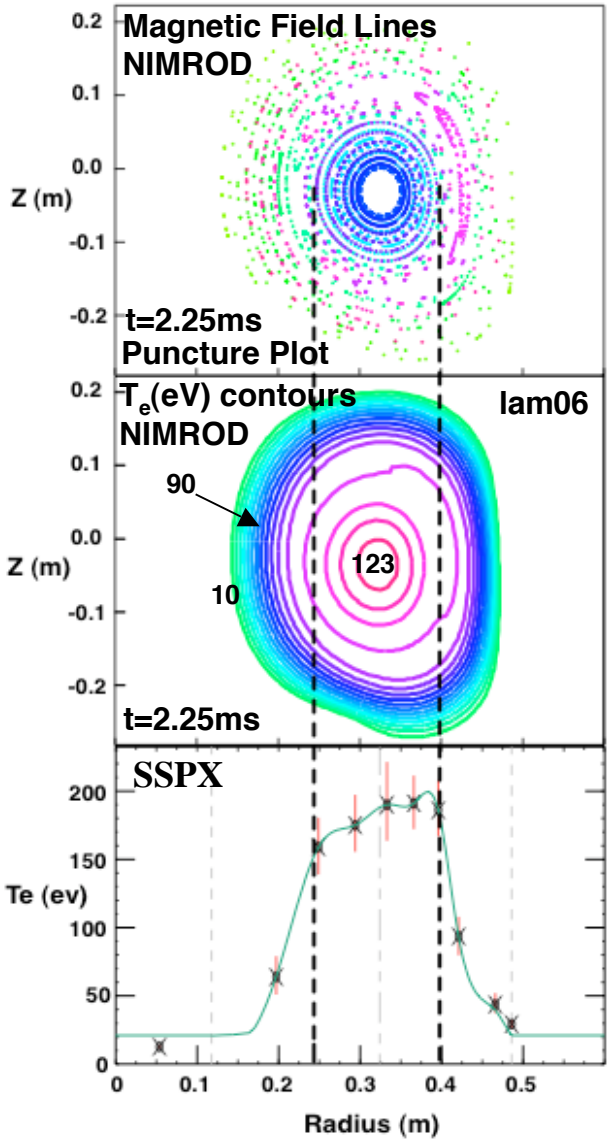
1. Include an additional review criterion to require that larger theory groups provide clear evidence of collaborative work and the extent to which the group addresses problems requiring a team effort
2. increase opportunities for new investigators
3. encourage greater interaction between the theory and experimental programs. We recommend that experimentalists be invited to participate in the peer review process for theory grants and that reviewer evaluation criteria include efforts to validate theoretical models.

The theory program has been responsive to the recommendations of the review committees

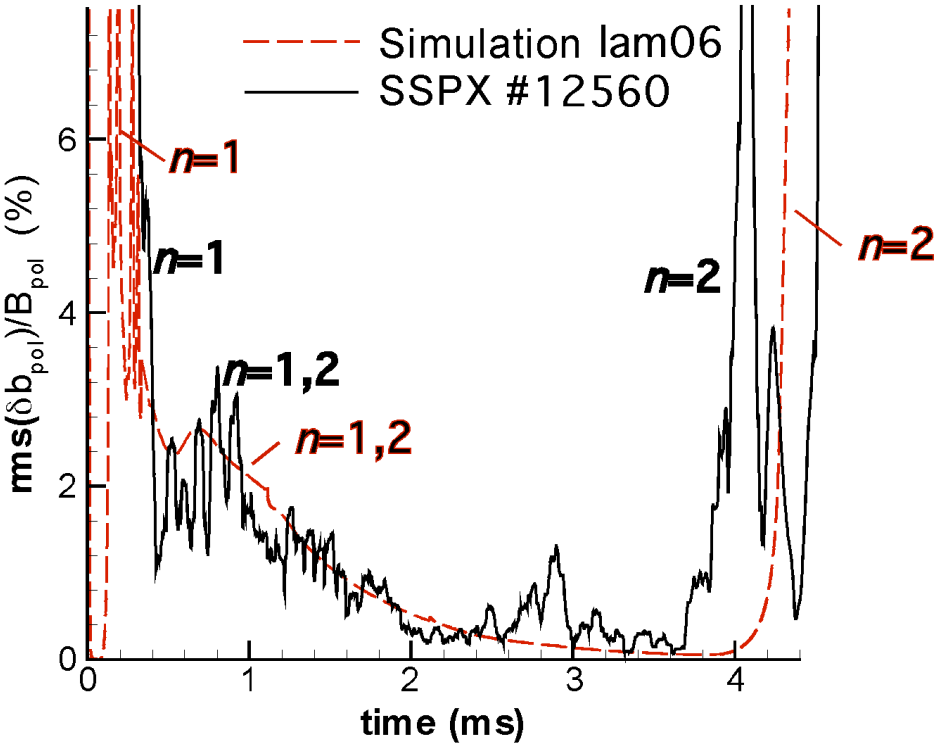
- Advanced computing strengthened through SciDAC centers, integrated simulation initiative
- Connectivity with non-fusion science enhanced through SciDAC, Fusion Science Centers
- Young scientists have created new fusion groups, often with the help of Young Faculty Awards program (Held, McCarthy, Newman, Rogers, Ware,…)
- Recommendations of COV panel have been adopted; peer review system improving

Recent Achievements

NIMROD simulations show striking similarities to SSPX experimental data for fluctuations and temperatures



Correlation of edge of "good field-line" region (NIMROD) with cliff in T_e (SSPX)

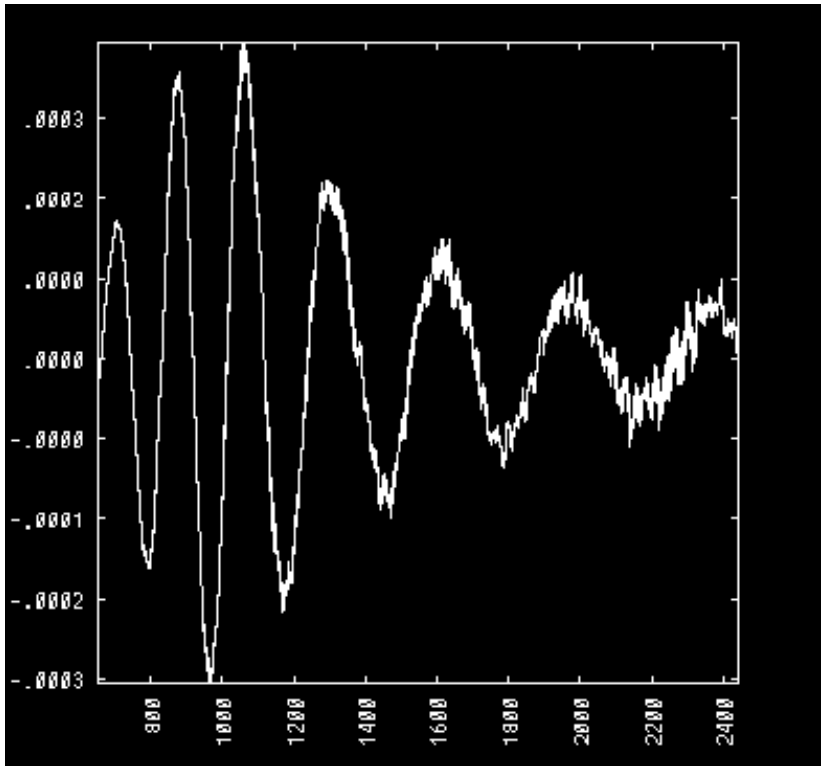


Similar fluctuation amplitude histories

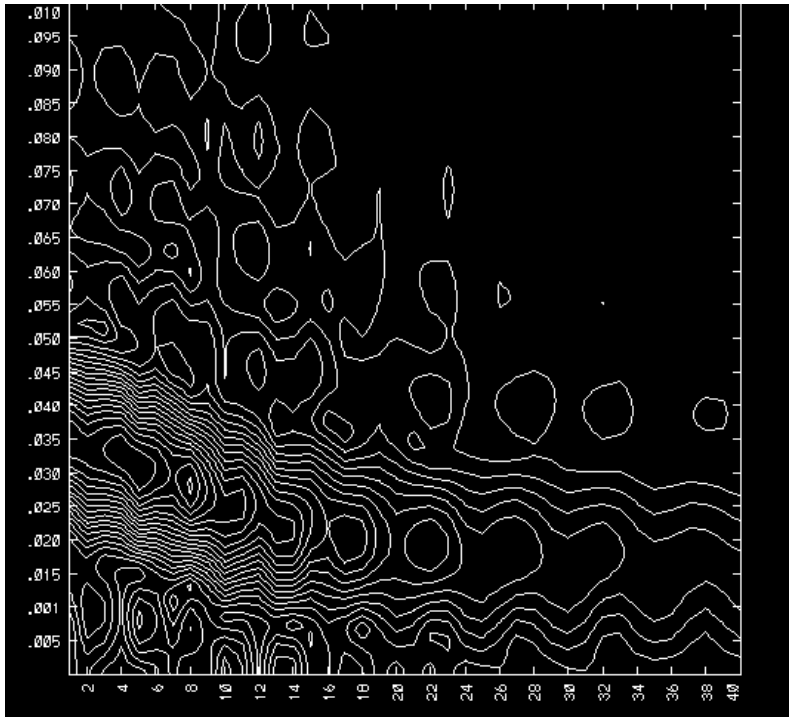
B. Cohen, E.B. Hooper, *LLNL*, C.R. Sovinec, *U. Wisc.*

Nonlinear simulation of fishbone shows strong frequency chirping

Nonlinear, fully self-consistent M3D simulations show that viscosity controls the relative role of kinetic (trapping) vs. fluid (Alfven resonance) nonlinearities



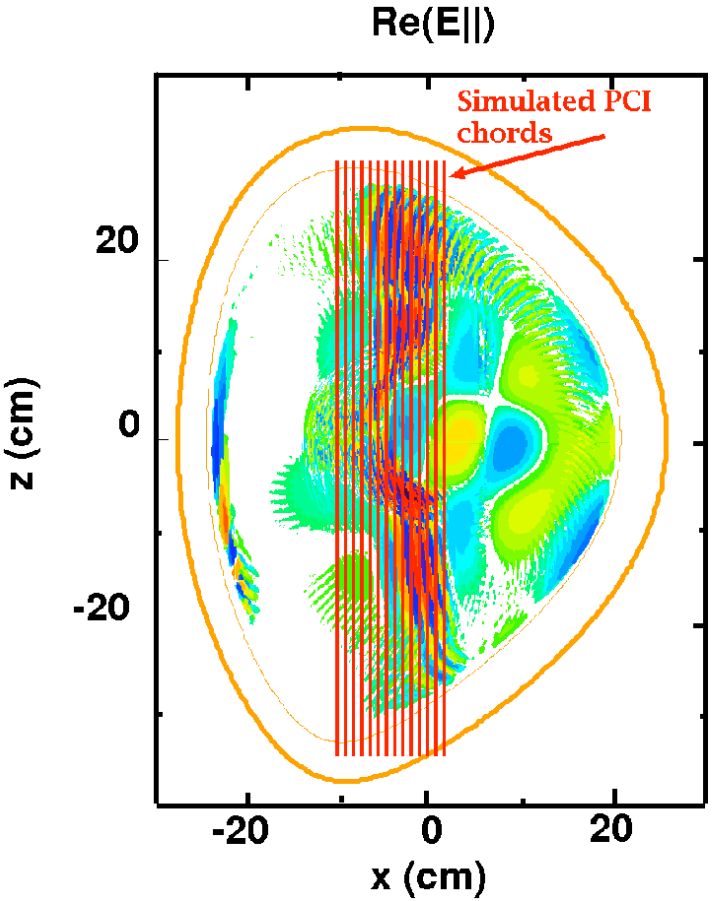
Amplitude v.s. time



Frequency v.s. time

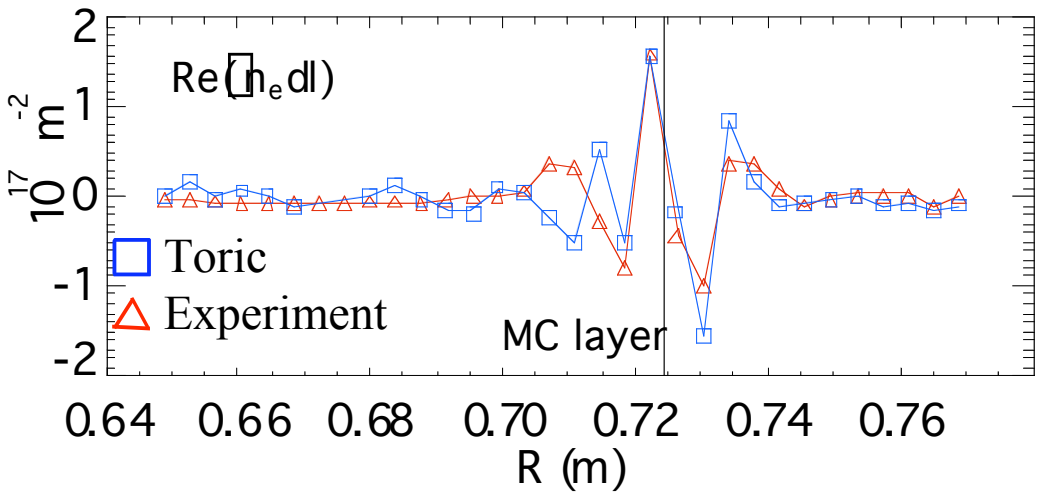
G.Y. Fu, PPPL

ICRF Synthetic PCI agrees well with Experiment



TORIC models the PCI on Alcator C-Mod that measures the perturbed density due to mode converted ICRF waves.

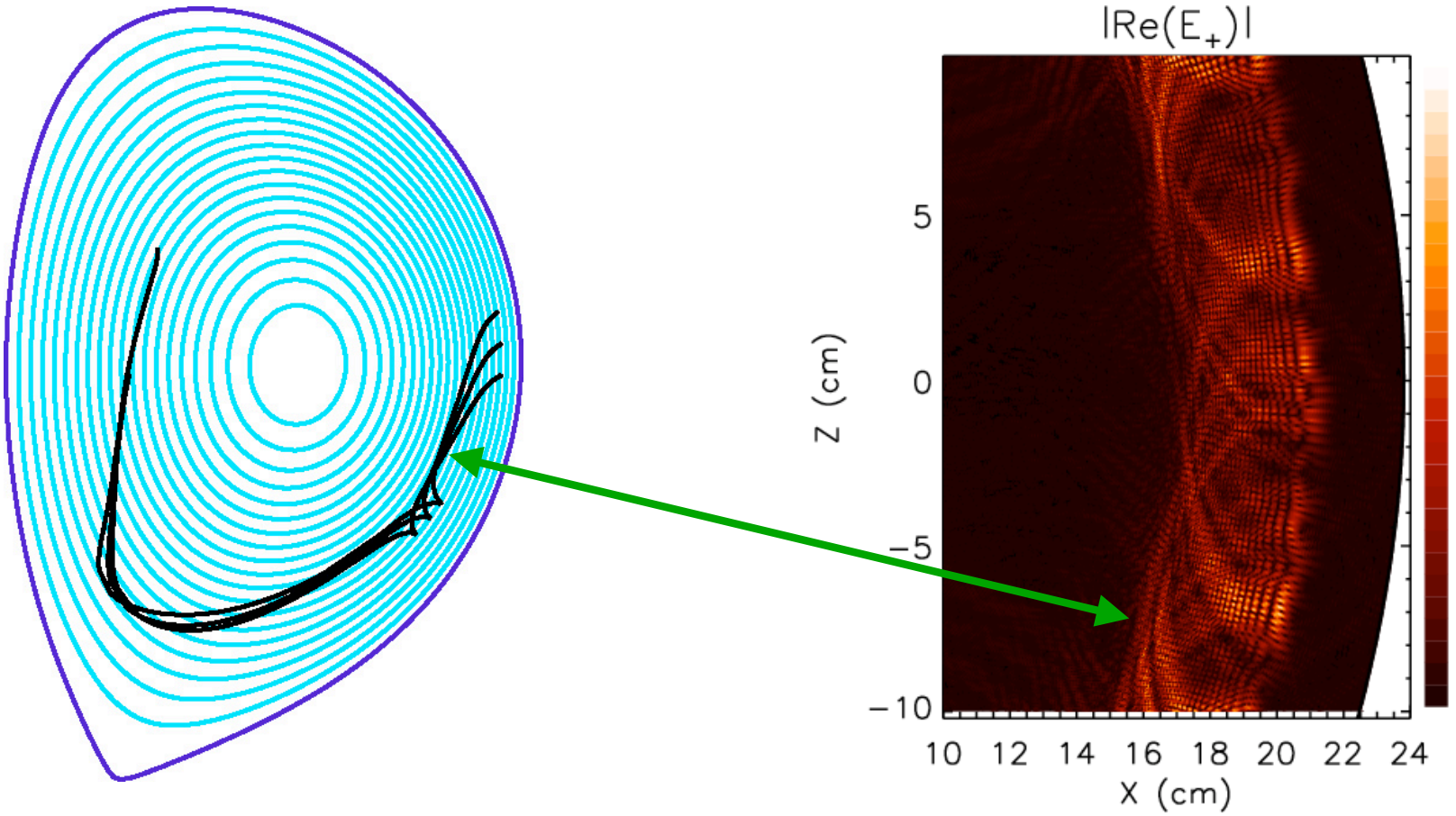
RF fluctuating density



- In agreement with Perkins 1977 theory describing MC into ICW vs. IBW
- The location and phase of the simulated signal agrees with the measured one.
- TORIC and the synthetic PCI are now used to interpret and plan Alcator C-Mod RF experiments.

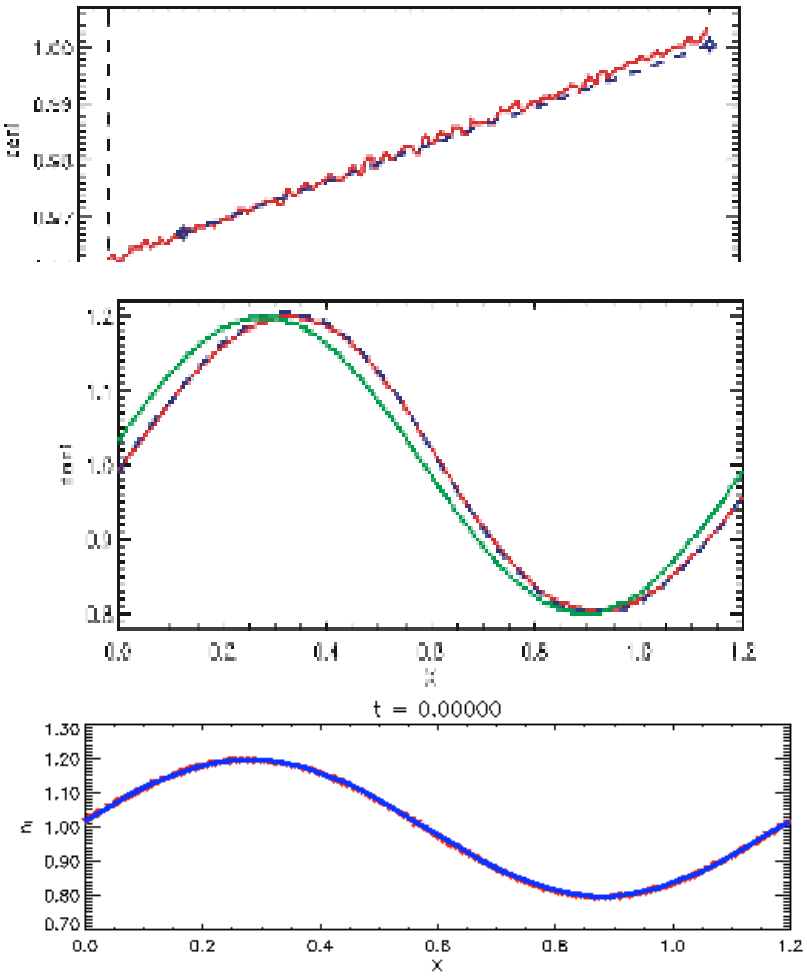
Y. Lin, A. Parisot, M. Porkolab, J. Wright, S. Wukitch

Full-wave LH caustic formation agrees with the ray tracing prediction



- After several reflections the rays penetrate to the plasma core, while the full wave fields are confined to the annulus shown above.
- Spectral broadening from diffraction occurs in the full wave results.

Projective integration shows promise for multiscale problems

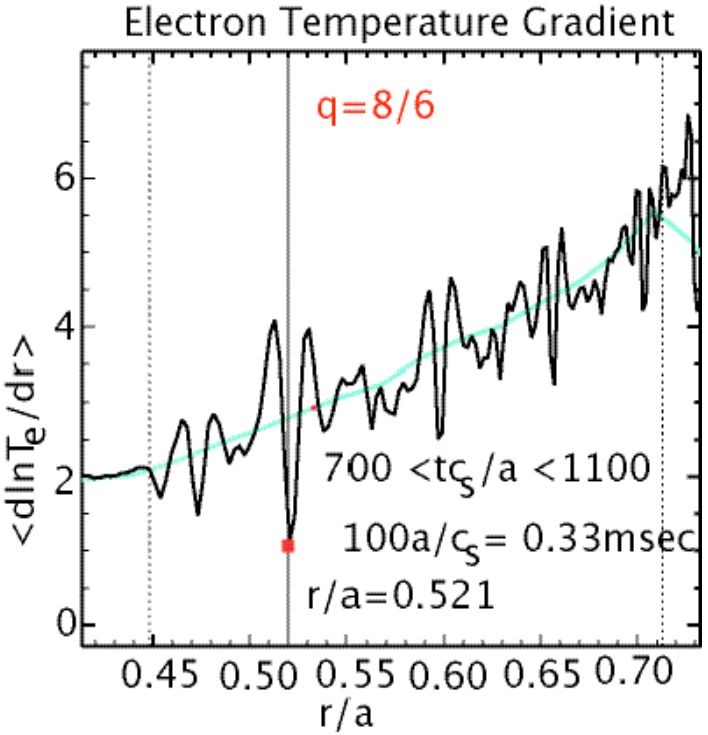


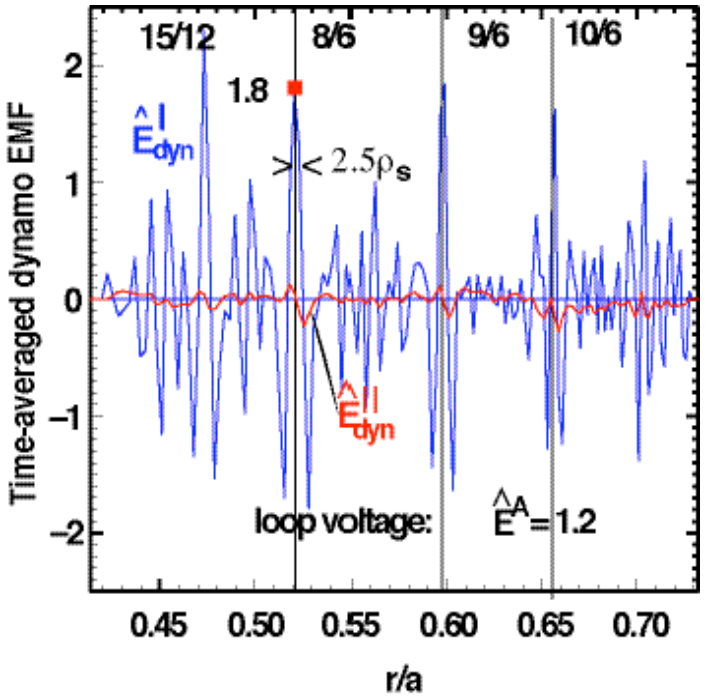
M. Shay 2005
U. MD & CMPD

- Center for Multiscale Plasma Dynamics held its first school and workshop at UCLA January 3-7 & 10-14 2005
- Key idea is to apply the projective integration technique of Kevrekedis and Gear to extend existing fusion codes
- Early tests show the method requires physics-guided adjustments but factor of 20 speedup of PIC code for ion-acoustic wave propagation problem are possible

Microturbulence creates profile corrugations that may affect long wavelength modes, such as tearing modes

- "Equilibrium" flux-surface averaged radial profiles of gradients (and divergences) are highly corrugated on the scale of a few ion gyroradii.
- The corrugations are "components of zonal flows" tied to low order singular surfaces



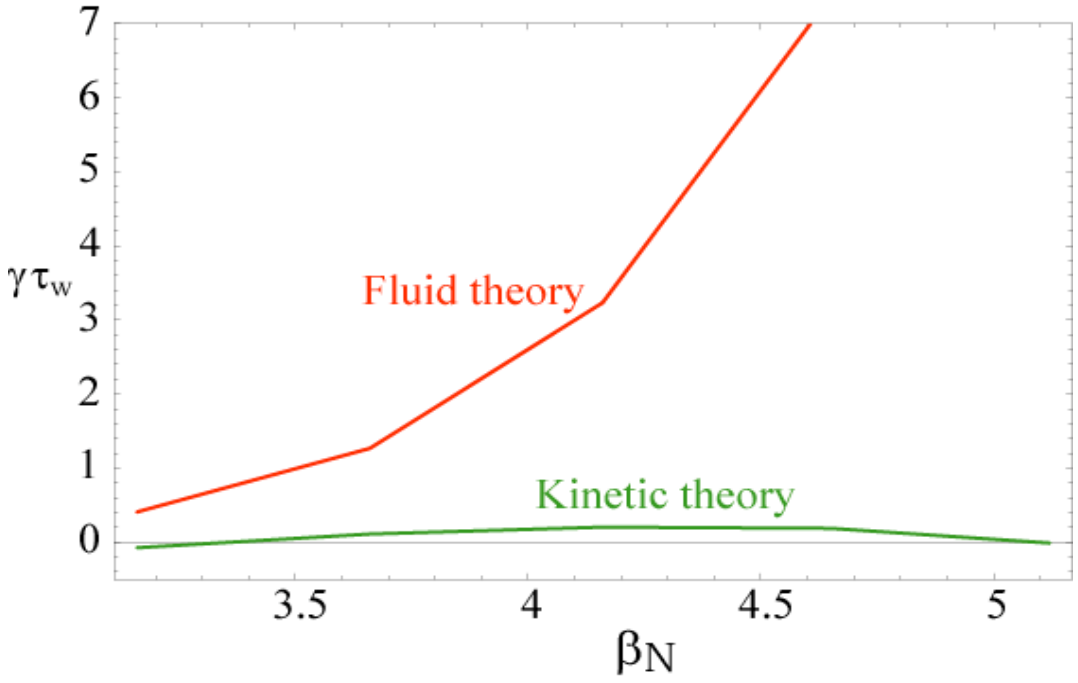


- **EMF(I) is from magnetic flutter (like the MHD □ - dynamo) and EMF(II) is electrostatic.**

J. Candy and R. Waltz, GA

Kinetic effects are stabilizing in tokamaks with low rotation - ITER

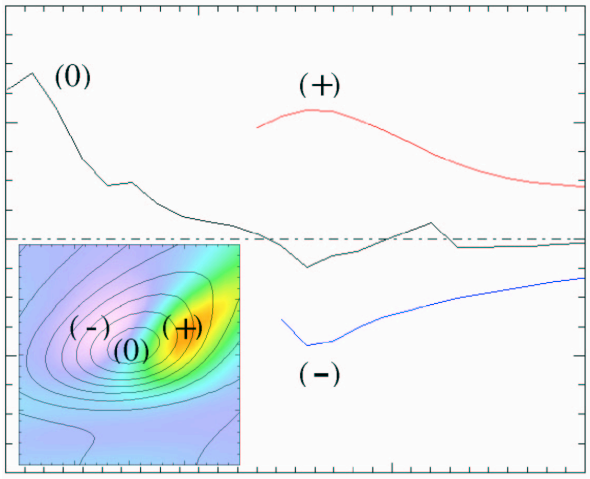
•ITER expected to rotate too slowly for conventional rotational stabilization of the resistive wall mode to be effective.
•For such low rotation, trapped particle compressibility and dissipation from the precession drift resonance are strongly stabilizing.

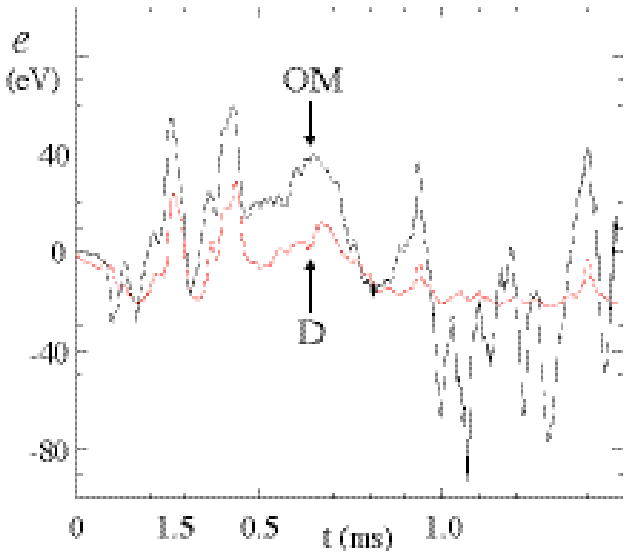


B. Hu, R. Betti, and J. Manickam,

U. Rochester and PPPL

BOUT simulations show decoupling from the edge during blob formation





- Blobs are monopolar density coherent structures that are electrically polarized
- 2D models of the SOL have used the sheath current-voltage relation to determine the current
- Recent results show that the potential on the outboard midplane decouples from that at the divertor due to the flattening of the blob by the magnetic shear.

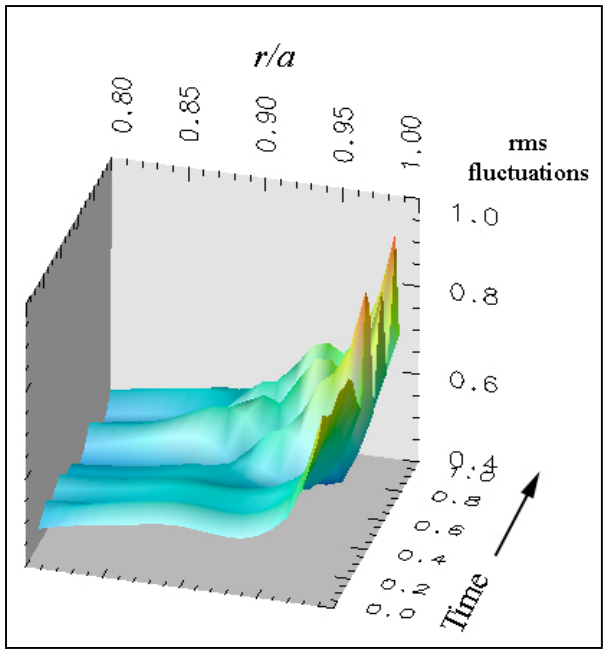
D. A. Russell, D. A. D X X Ippolito, J. R. Myra, W. M. Nevins, and X. Q. Xu, Lode Star and LLNL

Flow generation induced by a gas puff

- Edge shear flow generation induced by an increase in the particle source (modeling a gas puff) has been simulated and compared to observations in TJ-II experiments using the 1D transport model of D. Newman

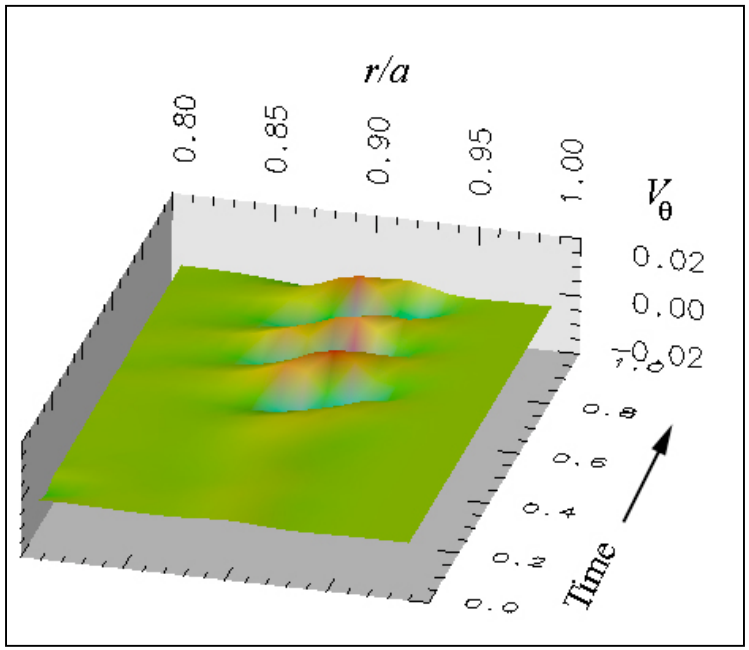
[C. Hidalgo, M. A. Pedrosa, L. Garcia, A. Ware, Phys. Rev. E (2004)]

Fluctuation level increases



As the particle source is ramped up, fluctuations increase (left) and an edge poloidal flow develops (right) through the Reynolds stress

Edge poloidal flow develops



Phys. Rev. Lett. papers give idea of overall production

- From March 04 -- Feb. 05 there were

Theory	Comp	Th/Xp	Xp/Th	Xp
5	4	1	9	12
10			9	12

•PRL gives distorted image of effectiveness in fusion program, but does play a significant role as our embassy to the wider physics community.

• Magnetic fusion PRL production is disturbingly small compared to other areas of plasma physics.

Theory program plays a central role in education

Princeton Plasma Courses Schedule AY 2002-2003

Fall 2002

AST 551	General Plasma Physics I	N.J. Fisch/ G. Hammett
AST 553	Plasma Waves and Instabilities	C.K. Phillips
AST 555	Fusion Plasmas and Plasma Diagnostics	P. Efthimion, R. Majeski, M. Zarnstorff
AST 557	Analytical Techniques in Differential Equations I	R.B. White
AST 558	Seminar in Plasma Physics	R.C. Davidson

Spring 2003

AST 552	General Plasma Physics II	W.M. Tang/ A. Reiman
AST 554	Irreversible Processes in Plasma	J.A. Krommes
AST 558	Seminar in Plasma Physics	N.J. Fisch / Stewart Zeben
AST 559	Turbulence in Fluids and Plasmas	J.A. Krommes
AST 560	Computational Methods in Plasma Physics	S.C. Jardin
AST 562	Laboratory in Plasma Physics	S.A. Cohen

(Cross-listed Courses).

Issues and challenges

Verification and validation Identified as key issue

(M. Greenwald, Comp. Phys. Commun. 2005)

- Verification concerned with fidelity of solution to mathematical model
- Validation is concerned with the fidelity of the model to reality

In CFD V&V is highly developed, commands vast resources.

Old adage, “the purpose of computation is to provide insight,” is inadequate. Computation is increasingly used to formulate *physical laws* (e.g. the scaling of the reconnection rate with the ion skin depth, the pedestal width with collisionality, etc…)

Resonance of the V&V question shows that the computing community is eager to move on from its excessive preoccupation with visualizations

TCC white paper addresses computing capability vs. capacity

- 42% of NERSC usage utilizes less than 256 of SEABORG's 6656 processors
- Productivity depends on turnaround time more than processing speed
- A mix of local clusters or cluster farms is needed to provide the most cost effective cycles/year.
- OFES has pledged support and has already funded a cluster at GA.

Some challenges require sustained attention

- Promoting interaction between theory, computing, and modeling
  - The challenge of maintaining connectivity will grow as the theory community is being sheared by the powerful attraction of computer science.
- Theoretical support of experiments
  - The data shows this is mostly a problem of perception. Increased interest in V&V should help
- More systematic management procedures
  - Role of TCC is growing but the committee needs to broaden its base and publicize its activities before it can fulfill the role envisaged in the Sheffield report.
- Integrated fusion simulation initiative is addressing issues of code portfolio management.

Conclusions

- Reviewing panels (Sheffield, Nevins) have judged the quality of the research in the T/C program to be high.
- The T/C program has been responsive to the program needs expressed by the reviewing panels.
- The T/C program has made progress in achieving the goals set by these panels.
- Funding retreats in SciDAC and Integrated Simulation Initiative are hurting our ability to benefit from progress in computation.
- The T/C program is making progress on the tasks identified by ITPA and the FESAC Priorities Panel. Today's theory program is laying the foundations for the prediction tools that will explain ITER and help design DEMO.